Explicit Higher Order Symplectic Integrator for s-Dependent Magnetic Field

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We derive second and higher order explicit symplectic integrators for the charged particle motion in an s-dependent magnetic field with the paraxial approximation. The Hamiltonian of such a system takes the form of $H = \sum_k (p_k - a_k(\vec{q}, s))^2 + V(\vec{q}, s)$. This work solves a long-standing problem for modeling s-dependent magnetic elements. Important applications of this work include the studies of the charged particle dynamics in a storage ring with strong field wigglers, arbitrarily polarized insertion devices, and super-conducting magnets with strong fringe fields. Consequently, this work will have a significant impact on the optimal use of the above magnetic devices in the light source rings as well as in next generation linear collider damping rings.

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I. INTRODUCTION

Symplectic integrators are a set of special numerical integration methods developed for the Hamiltonian systems. Unlike the more widely used Runge-Kutta algorithms which are non-symplectic in general, the symplectic integration methods allow numerical computations of the phase space vector at any time τ, $\{\vec{q}(\tau), \vec{p}(\tau)\}$, so that the transformation from the initial state, $\{\vec{q}(0), \vec{p}(0)\}$, to the final state, $\{\vec{q}(\tau), \vec{p}(\tau)\}$, is canonical. The early development of higher order (order ≥ 2) explicit symplectic integrators was initiated by Ruth's work for the following type of Hamiltonians [1]:

$$H = T(\vec{p}) + V(\vec{q}). \tag{1}$$

Applying the Lie map techniques, Forest [2] and Neri [3] re-derived Ruth's integrator, and found that such integrators were universally applicable to any Lie group. Later, Yoshida developed a systematic method [4] to construct higher even order integrators from a lower order one. This elegant piece of work eliminates the need to search for specific higher order integrators, for they can be iteratively constructed from a known second-order symplectic integrator. The further development by Forest extended the Yoshida's technique to the implicit integration and multi-map explicit integration [5] as well as for the time dependent Hamiltonians using the extended phase space concept [6].

In the storage ring, symplectic integration provides an essential tool to study the long-term behavior of the single particle dynamics. Magnetic multipole elements, such as quadrupoles and sextupoles, are modeled using a so-called impulse boundary approximation, in which the magnetic field is assumed to be constant (s-independent) within the effective boundary of the magnet and zero outside. Such a magnetic field model allows one to use a special vector potential, $\vec{A} = A_z(x, y)\hat{z}$ for each magnet. As a result, the charged particle Hamiltonian can be separated into the usual drift-kick combinations of the Ruth type: $H = T(\vec{p}) + V(\vec{q})$, where $T(\vec{p})$ is a drift, $V(\vec{q})$ is a kick. Applying the explicit symplectic integration method for magnetic multipoles developed in the early 1990's, it became possible to compute the charged particle trajectories after a large number of turns without introducing artificial damping or anti-damping. A number of tracking codes have since been developed with higher order symplectic integrators. These tracking codes have become a critical tool for designing the third generation light storage rings with small emittance as well as high energy physics collider rings with high luminosity.

However, in particle accelerators there are other types of magnetic elements, such as wigglers and undulators, their s-dependent magnetic field cannot be modeled properly by the above multipole model with the impulse boundary approximation. Consequently, the charged particle Hamiltonian can no longer be split into drift and kick combinations. Instead, the Hamiltonian for s-dependent magnetic fields takes the following form:

$$H = T(\vec{p} - \vec{a}(\vec{q}, s)) + V(\vec{q}, s). \tag{2}$$

This paper focuses on our recent development of higher order explicit symplectic integrators for such a Hamiltonian.

In section II, we state the mathematical problem to be solved. In section III, we revisit the Yoshida's procedures to iteratively construct higher order symplectic integrators. Explicit integrators are then developed in section IV for the s-dependent magnetic field Hamiltonian with the

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paraxial approximation. In section V we implement this type of integrator using a magnetic quadrupole as an example. Finally, we outline a few important applications of this work in section VI.

II. THE PROBLEM

The goal of this paper is to find explicit symplectic integrators for the charged particle Hamiltonian with an s-dependent magnetic field. A general static magnetic field depends on all three coordinates and can be described by a vector potential of the form, $\vec{A}(\vec{r}) = A_x(\vec{r})\hat{x} + A_y(\vec{r})\hat{y} + A_z(\vec{r})\hat{z}$, and $\vec{r} = (x, y, z)$. The Hamiltonian for such a field is,

$$\begin{aligned} & H(x, p_x, y, p_y, \delta, l; z) \\ & = -\sqrt{(1+\delta)^2 - (p_x - a_x)^2 - (p_y - a_y)^2} - a_z, \end{aligned} \quad (3)$$

where $p_{x,y} = P_{x,y}/P_0$ is the normalized transverse momenta, $\delta = P/P_0 - 1$ is the relative momentum deviation, l is the path length, $a_{x,y,z}(x, y, z) = qA_{x,y,z}(x, y, z)/(P_0 c)$ is the normalized vector potential.

Clearly, we observe that such a Hamiltonian always contains terms which mix the coordinate and momentum of the same canonical pairs, such as in $(p_{x,y} - a_{x,y}(x, y, z))^2$. Therefore, explicit symplectic integration techniques developed for Hamiltonians of the Ruth type are no longer applicable. This problem is particularly difficult, for the transverse momentum terms are grouped together under the roof of the square root.

In large rings, the paraxial approximation can be made for the charged particle motion. With this approximation, the Hamiltonian can then be simplified to the following form:

$$\begin{aligned} & H(x, p_x, y, p_y, \delta, l; z) \\ & \approx -\delta + \frac{(p_x - a_x)^2}{2(1+\delta)} + \frac{(p_y - a_y)^2}{2(1+\delta)} - a_z. \end{aligned} \quad (4)$$

Apparently, the mixing of the coordinate and momentum remains in this Hamiltonian. Many light source rings, damping rings, and collider rings fall into this category. Consequently, developing symplectic integrators for this reduced form of the Hamiltonian remains of great significance. In fact, by applying the generating function techniques, we find that this type of Hamiltonian can be broken into exactly solvable parts, therefore integrable by an explicit symplectic integration scheme (see section IV).

III. YOSHIDA'S PROCEDURE REVISITED

Consider a time independent Hamiltonian $H(\vec{q}, \vec{p})$, its Lie map from a time 0 to a time t can be symbolically written as,

$$\mathcal{M}(t) = \exp(t : -H :). \quad (5)$$

This Lie map cannot be evaluated exactly if the Hamiltonian is not solvable. Suppose that the Hamiltonian can be split into N solvable parts, $H = H_1 + H_2 + \cdots + H_N$, then, a second order integrator can be easily constructed using a symmetrized Lie map product [5]:

$$\begin{aligned} \mathcal{N}_i(t) &= \exp(t : -H_i :), \quad i = 1, \cdots, N \\ \mathcal{M}_2 &= \mathcal{N}_1(t/2)\mathcal{N}_2(t/2)\cdots\mathcal{N}_N(t)\cdots\mathcal{N}_2(t/2)\mathcal{N}_1(t/2) \\ &= \mathcal{M}(t) + O(t^3). \end{aligned} \quad (6)$$

Yoshida's method [4] allows one to systematically construct a higher-order integrator from a lower order one. Suppose that we have found a $2n$-th order symplectic approximation $\mathcal{M}_{2n}$ for $\mathcal{M}$. If $\mathcal{M}_{2n}(t)$ has the property of time reversibility, i.e. $\mathcal{M}_{2n}^{-1}(t) = \mathcal{M}_{2n}(-t)$, then $\mathcal{M}_{2n}(t)$ would only contain odd power terms of time, t, in its Lie exponent [6]. We can readily write $\mathcal{M}_{2n}(t)$ as

$$\mathcal{M}_{2n}(t) = \exp(: -tH + t^{2n+1}F_{2n+1} + O(t^{2n+3}) :). \quad (7)$$

Following Yoshida's procedure, one can construct an $(2n+2)$-th order integrator in the following way:

$$\begin{aligned} \mathcal{M}_{2n+2}(t) &= \mathcal{M}_{2n}(x_1 t)\mathcal{M}_{2n}(x_0 t)\mathcal{M}_{2n}(x_1 t) \\ &= \exp(: -t(2x_1 + x_0)H + \\ & \quad t^{2n+1}(2x_1^{2n+1} + x_0^{2n+1})F_{2n+1} + O(t^{2n+3}) :) \\ &= \exp(: -tH + O(t^{2n+3}) :). \end{aligned} \quad (8)$$

The last step is realized if we set

$$\begin{aligned} 2x_1 + x_0 &= 1 \\ 2x_1^{2n+1} + x_0^{2n+1} &= 0. \end{aligned} \quad (9)$$

One trivial real solution for the above equation is

$$x_1 = \frac{1}{2 - 2^{1/(2n+1)}}, \; x_0 = -\frac{2^{1/(2n+1)}}{2 - 2^{1/(2n+1)}}. \quad (10)$$

Because of Yoshida's recursive technique to construct higher order symplectic integrators, what left for us is to develop a second-order symplectic integrator for s-dependent magnetic field.

It is worth to note that since 1990's, mathematicians have actively involved in studying symplectic integration methods as part of geometric integration [7]. A wide range of research in this area has be published [8]. McLachlan's work on designing effective high-order integration methods [9] provides valuable insights to construct an optimal integrator for our problem.

IV. EXPLICIT SYMPLECTIC INTEGRATORS

The Hamiltonian for an s-dependent magnetic field explicitly depends on the independent variable s (or z in the Cartesian coordinate system, as in our case) (see Eq. 4). To facilitate the development of approximate Lie maps, we extend the phase space to include (z, p_z) as the fourth canonical pair and σ as an independent variable with $d\sigma = dz$ [6]. The equivalent paraxial Hamiltonian in the extended phase space is given by

$$\begin{aligned} & K(x, p_x, y, p_y, \delta, l, z, p_z; \sigma) \\ & \approx -\delta + \frac{(p_x - a_x)^2}{2(1+\delta)} + \frac{(p_y - a_y)^2}{2(1+\delta)} - a_z + p_z. \quad (11) \end{aligned}$$

Since this equivalent Hamiltonian is σ-independent, an exact Lie map for an integration step $\Delta\sigma$ can be written symbolically as:

$$\mathcal{M}(\Delta\sigma) = \exp(-\Delta\sigma : K :) \qquad (12)$$

Before constructing a second-order approximation for this map, we will make a gauge transformation so that the vector potential will have a zero component in the x-direction: $\vec{A} = A_y(x, y, z)\hat{y} + A_z(x, y, z)\hat{z}$. Now by splitting the Hamiltonian to several parts,

$$\begin{aligned} & K = K_1 + K_2 + K_3 + K_4, \qquad (13) \\ & K_1 = p_z, \quad K_2 = -a_z(x, y, z), \\ & K_3 = -\delta + \frac{p_x^2}{2(1+\delta)}, \quad K_4 = \frac{(p_y - a_y(x, y, z))^2}{2(1+\delta)}, \end{aligned}$$

we can construct a second-order approximation for $\mathcal{M}$ as follows:

$$\begin{aligned} & \mathcal{M}_2(\Delta\sigma) = \exp(: -\frac{\Delta\sigma}{2} K_1 :) \exp(: -\frac{\Delta\sigma}{2} K_2 :) \\ & \exp(: -\frac{\Delta\sigma}{2} K_3 :) \exp(: -\Delta\sigma K_4 :) \exp(: -\frac{\Delta\sigma}{2} K_3 :) \\ & \exp(: -\frac{\Delta\sigma}{2} K_2 :) \exp(: -\frac{\Delta\sigma}{2} K_1 :) \\ & = \mathcal{M}(\Delta\sigma) + O((\Delta\sigma)^3). \qquad (14) \end{aligned}$$

Apparently, K_1, K_2, K_3 are exactly solvable due to the separation of the coordinate and momentum belonging to the same canonical pairs while K_4 containing the (y, p_y) pair remains to be solved. However, using a generating function, we find that K_4 is also exactly solvable.

By noticing that K_4 contains only p_y but not p_x, a generating function is in order to transform $(p_y - a_y)^2$ to $(p_y^{\text{new}})^2$ using a set of new canonical variables. We write down the explicit Lie map for this generating function:

$$\begin{aligned} & \mathcal{A}_y = \exp(: -\int a_y(x, y, z) dy :), \qquad (15) \\ & \exp(: -\frac{\Delta\sigma(p_y - a_y)^2}{2(1+\delta)} :) = \mathcal{A}_y \exp(: -\frac{\Delta\sigma p_y^2}{2(1+\delta)} :) \mathcal{A}_y^{-1}. \end{aligned}$$

Transformations on the phase space variables by this generating function Lie map are explicit:

$$\begin{aligned} & \mathcal{A}_y\{x, y, z, \delta, l\} = \{x, y, z, \delta, l\}, \qquad (16) \\ & \mathcal{A}_y p_x = p_x - \int \frac{\partial a_y}{\partial x} dy, \ \mathcal{A}_y^{-1} p_x = p_x + \int \frac{\partial a_y}{\partial x} dy, \\ & \mathcal{A}_y p_y = p_y - a_y, \ \mathcal{A}_y^{-1} p_y = p_y + a_y, \\ & \mathcal{A}_y p_z = p_z - \int \frac{\partial a_y}{\partial z} dy, \ \mathcal{A}_y^{-1} p_z = p_z + \int \frac{\partial a_y}{\partial z} dy. \end{aligned}$$

Finally, we have completed the development of an explicit second-order symplectic integrator for $\mathcal{M}$:

$$\begin{aligned} \mathcal{M}_2(\Delta\sigma) = \; & \exp(: -\frac{\Delta\sigma}{2} p_z :) \exp(: \frac{\Delta\sigma}{2} a_z :) \exp(: -\frac{\Delta\sigma}{2}(-\delta + \frac{p_x^2}{2(1+\delta)}) :) \\ & \mathcal{A}_y \exp(: -\Delta\sigma \frac{p_y^2}{2(1+\delta)} :) \mathcal{A}_y^{-1} \exp(: -\frac{\Delta\sigma}{2}(-\delta + \frac{p_x^2}{2(1+\delta)}) :) \exp(: \frac{\Delta\sigma}{2} a_z :) \exp(: -\frac{\Delta\sigma}{2} p_z :). \qquad (17) \end{aligned}$$

It is worth pointing out that this particular second-order approximation for $\mathcal{M}$ is not unique. By choosing different magnetic field gauges for the vector potential, one can construct an infinite set of second order Lie map approximations which can be integrated explicitly. The construction of higher order symplectic integrators is trivial by following Yoshida's procedure outlined in section III.

V. QUADRUPOLE EXAMPLE

To illustrate the usage of this type of symplectic integrators, we use a magnetic quadrupole as an example. Traditionally, for magnetic multipoles, the vector potential is chosen with a A_z component only under the impulsed boundary approximation described in section I. For a quadrupole, $qA_z(x, y)/(P_0c) = -b_1/2(x^2 - y^2)$, and the Hamiltonian is,

$$H_1 = (-\delta + \frac{p_x^2 + p_y^2}{2(1+\delta)}) + \frac{b_1}{2}(x^2 - y^2) = H_1(\vec{p}) + H_2(\vec{q})$$
$$K_1(x, p_x, y, p_y, \delta, l; z) = H_1 + p_z, \quad (18)$$

where K_1 is the quadrupole Hamiltonian in the extended phase space. While this quadratic Hamiltonian is exactly solvable, a simple drift-kick separation of the Hamiltonian can be used for computing the particle trajectory numerically.

Now we choose a different field gauge so that the vector potential has a zero component in A_z:

$$\frac{q\vec{A}}{P_0 c} = (b_1 xz, -b_1 yz, 0), \quad (19)$$

and an equivalent Hamiltonian in the extended phase space is,

$$K_2 = \{-\delta + \frac{(p_x - b_1 xz)^2}{2(1+\delta)}\} + \{\frac{(p_y + b_1 yz)^2}{2(1+\delta)}\} + p_z$$
$$K_2 = \mathcal{A}_g K_1, \quad (20)$$

where $\mathcal{A}_g = \exp(: -\frac{1}{2} b_1 (x^2 - y^2) z :)$ is the Lie map for the relative gauge transformation between the two sets of vector potentials. Using generating functions, we transfer K_2 to a form with clearly recognizable solvable parts:

$$K_2 = \mathcal{A}_x(-\delta + \frac{p_x^2}{2(1+\delta)}) + \mathcal{A}_y(\frac{p_y^2}{2(1+\delta)}) + p_z, \quad (21)$$

where $\mathcal{A}_x = \exp(: -\frac{b_1}{2} x^2 z :)$ and $\mathcal{A}_y = \exp(: \frac{b_1}{2} y^2 z :)$.

Taking the above Hamiltonian (Eq. 21), we wrote a very simple second order symplectic integrator code. Using a differential algebra based package (FPP) of Forest we verified that the second-order quadrupole map was in fact symplectic. Then we tested this integrator on a very simple FODO lattice cell. We plot the phase space trajectories at the center of a defocusing quadrupole for 3000 turns in Fig. 1. Apparently, we observe that uncoupled horizontal and vertical phase space areas are conserved respectively, which once again demonstrates the symplectic nature of this integrator.

VI. CONCLUDING REMARKS

Although Ruth first speculated in 1980's [1] that an explicit high order map might be possible for a Hamiltonian of the form: $H = (\vec{p} - \vec{a}(\vec{q}, t))/2$, the exact procedure to construct such a high order symplectic integrator became evident only after Yoshida's work [4] and Forest's extension [6] to multi-maps in the extended phase space. The development of this explicit symplectic integrator for s-dependent magnetic field is very critical for understanding the single particle beam dynamics in the next generation storage rings, from light source rings to linear collider damping rings.

Two types of applications are particularly important. The first type is the modeling of fringe field dominated super-conducting magnets in storage rings. Superconducting dipoles and wavelength shifters are increasingly becoming a preferred radiation source for hard x-rays in some third generation light source rings. The Advanced Light Source (ALS) will commission three superconducting bending magnets in the fall of 2001. The s-dependent magnetic field in such devices can be properly modeled using an explicit symplectic integrator described in this paper.

The second type of applications is the modeling of magnetic undulators and wigglers, both linearly or elliptically polarized. Until recently, the most comprehensive wiggler modeling was performed by the BESSY group using the generating function based implicit method [10], [11], [12]. In this method, a symplectic higher order map was produced numerically for the insertion device. However, besides the convergence issues and limited order of the map which can be produced, the implicit method has difficulties in dealing with parameter-dependency of the field, and is limited to producing maps for a given design orbit. The explicit method developed here allows the generation of canonical maps with any parameter dependency by tracking through a magnet once with a differential algebra package. More importantly, since the method is explicit in nature, direct trajectory tracking in the real magnetic field can be performed for dynamic aperture studies. Consequently, this provides a benchmark for the dynamics studies in which the large amplitude motion may or may not be properly described by the on-axis map at a pre-determined order. This is particularly important for the wiggler dominated storage rings such as the next generation linear collider damping rings.

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VII. FIGURES

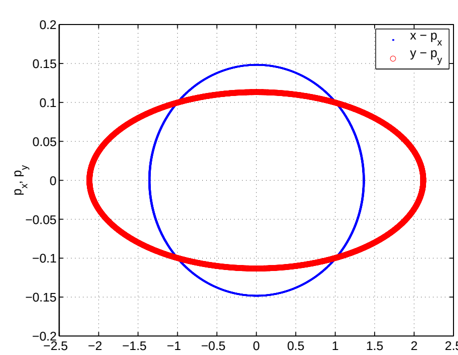

FIG. 1: A simple phase space trajectory plot for a FODO lattice at the center of a defocusing quadrupole (3000 turns). Quadrupole parameters are, l_q= 0.1, $(b_1)_{\mathrm{f}}$ = 2.2, $(b_1)_{\mathrm{d}}$ = −2.0. The drift length is $l_d = 0.2$.

APPENDIX A: GAUGE TRANSFORMATION AND ITS LIE MAP

Any given static magnetic field, $\vec{B}$, can be computed via a vector potential, $\vec{B} = \nabla \times \vec{A}_1$ for static magnetic field [13]. Because of the freedom of gauge transformations, there are a set of infinite equivalent vector potentials for the same magnetic field. Let us construct an equivalent vector potential for $\vec{A}_1$ using a gauge transformation:

$$\begin{aligned} &\vec{A}_2 = \vec{A}_1 + \nabla\Phi \\ &\nabla \times \vec{A}_2 = \nabla \times \vec{A}_1 = \vec{B}, \end{aligned} \tag{A1}$$

where Φ is an arbitrary analytic function.

Now, we can write two equivalent Hamiltonians, $H_{1,2}(x, p_x, y, p_y, \delta, l; z)$, for the same charged particle motion using $\vec{A}_1$ and $\vec{A}_2$,

$$\begin{aligned} H_1 &= -\sqrt{(1+\delta)^2 - (p_x - a_{x1})^2 - (p_y - a_{y1})^2} - a_{z1}, \\ H_2 &= -\sqrt{(1+\delta)^2 - (p_x - a_{x2})^2 - (p_y - a_{y2})^2} - a_{z2}, \end{aligned} \tag{A2}$$

see variable definitions in section II. These two equivalent Hamiltonians, are related by a canonical transformation. In fact, an explicit Lie map for the transformation can be written in terms of the gauge function, Φ,

$$\begin{aligned} &\mathcal{A}_g = \exp(: -\phi(x, y, z) :) \\ &H_2 = \mathcal{A}_g H_1, \end{aligned} \tag{A3}$$

where $\phi = q\Phi(x, y, z)/(P_0 c)$.

One important observation is that for any static magnetic field, one of the vector potential components can be set to zero by choosing a proper gauge. For example, by choosing a Φ such that $\frac{\partial\Phi}{\partial z} = -A_{z1}$, we can zero A_{z2}, resulting in an equivalent $\vec{A}_2 = (A_{x2}, A_{y2})$. This observation is very useful in constructing an efficient symplectic integrator.

Another observation is that the gauge transformation provides the continuity of the mechanical momenta. At the boundary of the transformation, applying the gauge transformation map, $\mathcal{A}_g$, to the phase space variables yields:

$$\mathcal{A}_g(p_\sigma - a_{\sigma 1}) = p_\sigma - a_{\sigma 1} - \frac{\partial\phi}{\partial\sigma} = p_\sigma - a_{\sigma 2}, \tag{A4}$$

where $\sigma = (x, y, z)$.

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